Elasticity of entangled polymer liquids : from F-actin to polyethelyne via primitive path anaylsis(Poster session 1, New Frontiers in Colloidal Physics : A Bridge between Micro- and Macroscopic Concepts in Soft Matter)

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概要： からみあった高分子系のプラトー弾性率は平衡状態における原始経路の配位から知ることができる。我々は、計算機シミュレーションによる原始経路の解析とスケーリング理論を組み合わせることにより、柔らかい合成高分子から硬い生体高分子にわたるからみあい高分子系の平衡状態についての統一的な描像を提供する。我々の得た弾性率の表式は、剛直性や密度の広い範囲にわたって実験結果とよく一致する。

The rheology of concentrated polymer solutions and melts are analyzed on the idea that entanglements confine individual chains to a one-dimensional, tube-like regions. While this picture has been extensively applied to loosely entangled flexible polymers, less attention has been paid to tightly entangled semiflexible polymers, which are biologically important. Here we combine computer simulations and scaling arguments to develop a unified view of polymer entanglement based on primitive path analysis (PPA).

Primitive paths are the shortest paths between the end-points of each chain that are topologically equivalent to the original chain configuration. This can be numerically implemented by fixing the end-points and then contracting the chain contours without crossing each other [1,2]. resulting in a mesh of mutually entangled, piecewise straight lines (primitive paths). To them we apply the theory of entangled semiflexible chains [3] regarding the PPA as a means to renormalize the loosely to a tightly entangled system. In particular, the plateau modulus G_N^0 is given by:

$$G_N^0 = C_G(k_BT/\ell_K^3)(\rho_K\ell_K^3)^{7/5}(L'/L)^{8/5}$$

where ℓ_K and ρ_K are the length and number density of the Kuhn segments, while L and L' are the (average) lengths of the original chains and the primitive paths. We used two types of model polymer liquids: tightly entangled solutions of zero-diameter WLCs with $10 < \rho_K\ell_K^3 < 10^5$ [2] and dense melts of flexible bead-spring chains with $1 < \rho_K\ell_K^3 < 40$ [1]. The chain contraction ratio L/L' is obtained from the numeical PPA to estimate the plateau modulus, which are compared with experimental data for semiflexible biopolymers (actins, fd-phages) and also synthetic flexible polymers. With $C_G = 0.2$, we find excellent agreement between the experimental data and our results over 5 decades in the dimensionless segment density. We also develop an approximation formula for L'/L which gives a two-parameter fitting of the plateau modulus.

References

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